

# Two-atomic potential and distortion of excitation spectrum of liquid $^4\text{He}$ by admixture of $^3\text{He}$

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## ABSTRACT

The new interatomic potential  $g(r)$ , providing the tunnelling of atoms, is suggested for calculating HFB phonon-roton spectrum  $E(p)$  of liquid  $^4\text{He}$ . The tunnelling enables the calculations to reproduce the experimental dependence of shifts  $E(p)$  on pressure  $P$  induced by  $^3\text{He}$  admixture in the constant total density and volume.

Distortion of the excitation spectrum of liquid  $^4\text{He}$  by admixture of  $^3\text{He}$  was investigated experimentally in [1]. The authors of [1] appealed to the theoreticians to calculate the excitation spectrums in liquid-helium mixtures in order to explain their data. The first attempt [2] to explain the  $^4\text{He}$  spectrum shift theoretically was based on the primary experimental results [3], that were revised in [1] however. The recent theory [4] suggested a new version of interatomic potential and presented the calculation of  $^4\text{He}$  spectrum shift caused by admixture of  $^3\text{He}$ . Still the result [4] disagreed with the experiments [1], the explanation of that could be supposed in the invalidity of Hartree-Fock-Bogoliubov approximation (HFB) in [4]. Now we try to improve the situation using a more realistic potential than that in [4] in the framework of HFB approximation. We show that the experimental data can be explained by postulating that the realistic potential curve differs from the usually assumed potential curve: the realistic potential has a local repulsive maximum in the attractive region of the usual curve. Moreover, the potential depends of the pressure (see Fig.1).

In this paper, we present an interaction potential  $U$ , providing the tunnelling of atoms through the local maximum. This property is inherent for the atoms in liquids and fills the gap between discrete and continuous spectrums of ordinary two-atomic potential.

Following [5], we assume that the polarization effects are not important in the liquid  $^4\text{He}$  and calculate the interaction potential  $U$  between two  $^4\text{He}$  atoms with electrons in the ground state. We use the formula for the interaction energy of two atoms with charge distributions densities  $\rho_1(\mathbf{r})$  and  $\rho_2(\mathbf{r})$

$$U = \int \frac{\rho_1(\mathbf{r})\rho_2(\mathbf{r}')d\mathbf{r}d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|}, \quad (1)$$

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where the charge densities are

$$\begin{aligned}\rho_1(\mathbf{r}) &= q\delta(\mathbf{r} - \mathbf{r}_1) - qF(\mathbf{r} - \mathbf{r}_1), \\ \rho_2(\mathbf{r}') &= q\delta(\mathbf{r}' - \mathbf{r}_2) - qF(\mathbf{r}' - \mathbf{r}_2).\end{aligned}\tag{2}$$

Here  $F(\mathbf{r} - \mathbf{r}_1)$  and  $F(\mathbf{r}' - \mathbf{r}_2)$  are the electron probability densities at the points  $\mathbf{r}$  and  $\mathbf{r}'$ , the atom nuclei being at the points  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , and  $q = 2e$ . The interaction between atoms contains three terms:  $U_{nn}$ ,  $U_{nc}$ ,  $U_{cc}$ , describing interactions between two nuclei, nucleus of one atom with the cloud of the another and between two clouds.

The term  $U_{nc}$  has the form

$$U_{nc} = -q^2 \int \frac{\delta(\mathbf{r} - \mathbf{r}_1)F(\mathbf{r}' - \mathbf{r}_2)d\mathbf{r}d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} = -q^2 \int \frac{F(\mathbf{r}' - \mathbf{r}_2)d\mathbf{r}'}{|\mathbf{r}_1 - \mathbf{r}'|} = -q^2 \int \frac{F(\mathbf{r}_0)d\mathbf{r}_0}{|\mathbf{R} - \mathbf{r}_0|}, \tag{3}$$

where  $\mathbf{r}_0 = \mathbf{r}' - \mathbf{r}_2$  and  $\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2$  is a 3D vector between nuclei. The electron probability density  $F(r)$  is determined by the electron wave function  $\Phi$  of the  $^4\text{He}$  atom. Therefore we use the Hylleraas-type wave function with parameters  $\gamma_{1,2}$  (see [6])

$$\begin{aligned}\Phi &= e^{-s/2a} \left( 1 + \gamma_1 \frac{u}{a} + \gamma_2 \frac{t^2}{a^2} \right), \quad s = r_3 + r_4, \\ t &= r_3 - r_4, \quad u = |\mathbf{r}_3 - \mathbf{r}_4|,\end{aligned}$$

where  $\mathbf{r}_3$  and  $\mathbf{r}_4$  are the electron coordinates of atoms  $a$  is the Bohr radius. In order to obtain the probability density (2) of the cloud  $F$  at the point  $r$  one can add the  $w_1$  and  $w_2$  probabilities to find one electron at the point  $r$ , and another at an arbitrary point

$$qF(r) = ew_1(r) + ew_2(r),$$

$$w_1(r) = \int |\Phi(\mathbf{r}_3 = \mathbf{r}, \mathbf{r}_4)|^2 d\mathbf{r}_4, \quad w_2(r) = \int |\Phi(\mathbf{r}_3, \mathbf{r}_4 = \mathbf{r})|^2 d\mathbf{r}_3,$$

These expressions show, that the probability density  $F(r)$  can be written as

$$F(r) = \frac{1}{\pi a^3} e^{-2r/a} (\alpha_4 r^4 + \alpha_3 r^3 + \alpha_2 r^2 + \alpha_1 r + \alpha_0 + \alpha_{-1} \frac{1}{r}) = \frac{1}{\pi a^3} e^{-2r/a} \psi. \tag{4}$$

Thus, the formula for  $U_{nc}$  is

$$U_{nc} = -\frac{q^2}{\pi a^3} \int \frac{e^{-2r_0/a} \psi(\mathbf{r}_0) d\mathbf{r}_0}{|\mathbf{R} - \mathbf{r}_0|}. \tag{5}$$

The direct computations give

$$\begin{aligned}U &= \text{const} \cdot e^{-2x} \cdot \left( \beta_6 x^6 + \beta_5 x^5 + \beta_4 x^4 + \beta_3 x^3 + \right. \\ &\quad \left. + \beta_2 x^2 + \beta_1 x + \beta_0 + \beta_{-1} \frac{1}{x} \right), \quad x = \frac{R}{a}.\end{aligned}\tag{6}$$

The parameters  $\alpha$  in (4) are the functions of parameters  $\beta$  in (6). We emphasize that the potential (6) decreases exponentially at the distances  $R \gg a$ .

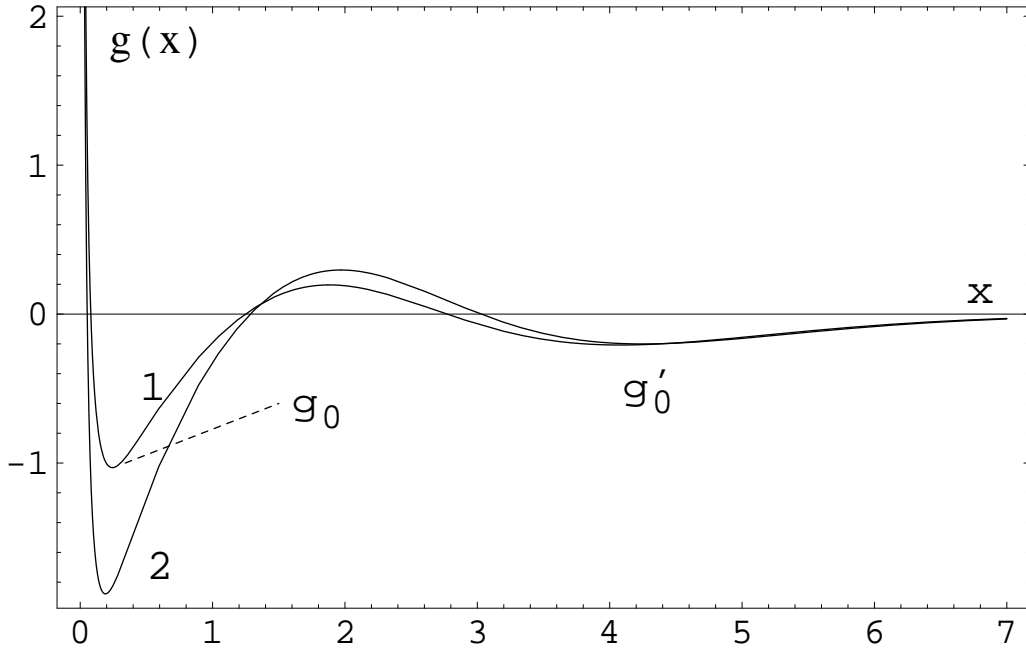


Fig. 1: Initial (1) and shifted (2) potential  $g(x)$ .

For the sake of simplicity, we limit ourselves by considering the potential of the form

$$g(x) = \text{const} \cdot e^{-2x} \left( Ax^6 + Bx^5 + C + D\frac{1}{x} \right), \quad (7)$$

instead of  $U(x)$ ;  $g(x)$  has the local maximum and depends on the minimum number of parameters (see Fig. 1).

It was shown in [1], that the pressure  $P$  increase in  $^4\text{He}$  due to the  $^3\text{He}$  admixture (in the same volume  $V$  and for the same total atomic density) leads to the deformation of phonon-roton  $^4\text{He}$  excitation spectrum  $E(p)$ . Our purpose is to reproduce the deformation  $\Delta(E) = E(p)|_P - E(p)$  of spectrum curves caused by the pressure  $P$ . The HFB formula for the spectrum of noncondensate excitation is

$$E(p) = \sqrt{\frac{p^4}{4m^2} + \frac{p^2}{m}\rho\tilde{g}(p)},$$

where  $m$  is the mass of atom,  $\rho$  is the condensate density and  $\tilde{g}$  is the Fourier transform of  $g$ . The increase of  $P$  leads to decrease of  $\rho$  and to the deformation of the electron clouds of the atoms, which keep, however, spherically symmetric. This is evident that the cloud deformation results in the displacement of the potential minimum  $g_0$  "down" and "to the left" in the  $x, g(x)$  plane. These curves 1,2 are shown in Fig. 1 and corresponds the values

$$A_1 = -0.5, B_1 = 1.4, C_1 = -2.5, D_1 = 0.2,$$

$$A_2 = -0.59, B_2 = 1.8, C_2 = -3.8, D_2 = 0.2.$$

The choice of parameters  $A, B, C$  and  $D$  is determined by the conditions for the potential: to be positive (repulsive) for  $x \ll 1$  ( $D > 0$ ), to be negative (attractive) for  $x \gg 1$  ( $A < 0$ ), to have local maximum.

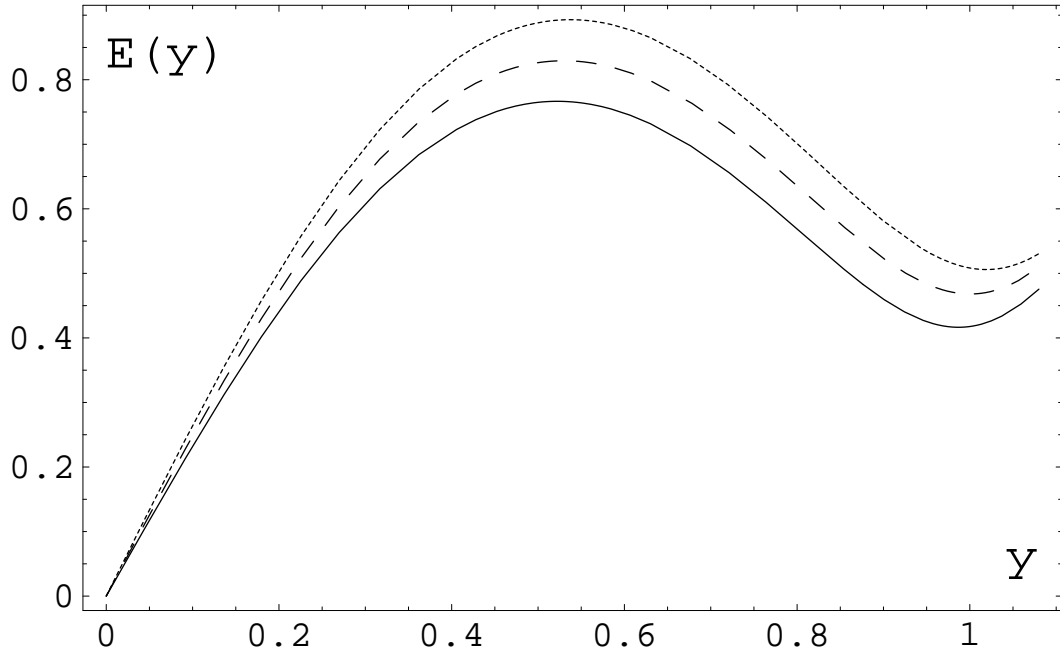


Fig. 2: Shift of  $E(y)$  with the change of parameters:  $A = -0.5$ ,  $B = 1.4$ ,  $C = -2.5$ ,  $D = 0.2$ ,  $\tilde{\rho} = 0.03$  (solid line);  $A = -0.59$ ,  $B = 2.3$ ,  $C = -19$ ,  $D = 0.2$ ,  $\tilde{\rho} = 0.027$  (dashed line);  $A = -0.61$ ,  $B = 4.5$ ,  $C = -30$ ,  $D = 0.2$ ,  $\tilde{\rho} = 0.025$  (dotted line).

The local maximum of  $g(x)$  occurs between coordinates of  $g_0$  and  $g'_0$ . This maximum is introduced in order to describe the tunnelling of atoms, providing the agreement of the present calculation with the experimental results for  $\Delta(E)$  in [1]. This tunnelling was not taken into account in [4], and this is the reason for a failure of [4] to explain [1].

In order to calculate the spectrum, we need the Fourier transform of  $g(x)$

$$\begin{aligned} \tilde{g}(y) &= -const \cdot a^3 \int_0^\infty \frac{\sin xy}{xy} g(x) x^2 dx = \\ &= -const \cdot a^3 \left[ A\Gamma(8)(4+y^2)^{-4} \sin[8 \arctan(y/2)] + B\Gamma(7)(4+y^2)^{-7/2} \sin[7 \arctan(y/2)] + \right. \\ &\quad \left. + \frac{4C}{(4+y^2)^2} + \frac{D}{(4+y^2)} \right], \quad \text{where } y = ap. \end{aligned}$$

We let  $g_0$  and  $g'_0$  denote the minima of the potential  $U(x)$  (see Fig. 1), and consider the behavior of  $U(x)$ . The curves 1 and 2 in Fig. 1 demonstrate the general situation.

In order to obtain the experimental scale of spectrum shifts we use the Fourier images of potentials similar to Fig. 1, but different from them in scale. Energy excitation spectra for such potentials are shown in Fig. 2. The shifted curves (dashed, dotted) in Fig. 2 correspond the decrease of condensate density  $\rho$  and increase of pressure  $P$ , relative to the initial state (solid curve). The shifts of the curves in Fig. 2 qualitatively correspond the deformations of  $g(x)$  shown in Fig. 1.

The two types of shifts of initial curve are possible. If the potential has a local maximum, then there are no intersections of  $E(p)$ . We emphasize that if the potential has not a local maximum, then we obtain the intersections of the shifted spectrum curves as shown in [5].

The local maximum implies the tunnelling of atoms and we conclude that this property is inherent for quantum liquid. It means, that in the case of ordinary Lennard–Jones potential there are discrete and continuous parts of spectrum only. In our case the tunnelling of atoms is possible in the range of energies intermediate between continuous and discrete spectrum. This tunnelling enables us reproduce the experiment sign of  $\Delta(E)$ . It describes the atoms, penetrating in liquids through the energy gap corresponding the regimes of "nearest atoms ordering" (in solids) and "atomic distant disorder" (in gas).

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